

# Effect of spin-orbit impurity scattering in the superconducting state of $t - J$ model

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We study the effect of magnetic impurities in the  $d_{x^2-y^2}$ -wave superconducting (SC) state of the two dimensional  $t - J$  model. The spin-orbit and the spin-exchange interactions are examined by treating the impurity as a classical spin. The Bogoliubov de Gennes equation derived within a slave-boson mean-field approximation is solved numerically at  $T = 0$ . The spin-exchange scattering induces spin-triplet  $p$ -wave SC order parameters near the impurity, while a SC state with broken time-reversal symmetry and a spontaneous current appears in the presence of the spin-orbit interaction. When both interactions coexist, it turns out that a state which carries a spontaneous spin current occurs.

**KEYWORDS:**  $d$ -wave superconductivity,  $t - J$  model, Bogoliubov de Gennes equation, magnetic impurity, spin current

The symmetry of the superconducting (SC) states in high- $T_c$  cuprates has been studied intensively, and now it is established that the state has a predominantly  $d_{x^2-y^2}$ -wave character with a possible mixture of an  $s$ -wave component due to the orthorhombic lattice distortion in some systems.<sup>1)</sup> Recently the effect of nonmagnetic (Zn) and Magnetic (Ni) impurities in high- $T_c$  superconductors are of particular interest both theoretically and experimentally. This is because the effects of randomness in such unconventional superconductors can be quite different from those in conventional superconductors.

The low-energy electronic states of high- $T_c$  cuprates can be described by the  $t - J$  model on a square lattice.<sup>2,3)</sup> Mean-field (MF) theories based on a slave-boson method predict a superconducting state with a  $d_{x^2-y^2}$ -symmetry.<sup>4,5)</sup> They may also explain the magnetic<sup>6,7)</sup> as well as the transport<sup>8)</sup> properties of these systems if the gauge fields representing the fluctuations around the MF solutions are taken into account. The effect of nonmagnetic impurities in the SC state of this model has been examined by several authors.<sup>9,10,11)</sup>

In this article we study the effect of a magnetic impurity in the superconducting state of the  $t - J$  model by taking into account both the spin-exchange and the spin-orbit interactions between electrons and an impurity spin. We consider the case of single impurity (located at a site 0), assuming that the concentration of impurities is low so that their effect can be treated independently. In this work the impurity spin is treated as classical, i.e., the Kondo effect will not be considered.

The Hamiltonian of our system is

$$\begin{aligned}
 H = & - \sum_{\langle i,j \rangle, \sigma} t_{ij} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + h.c.) \\
 & + \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j - \mu \sum_{i\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma} \\
 & + V_0 \sum_{\sigma} \tilde{c}_{0\sigma}^\dagger \tilde{c}_{0\sigma} + J_0 \sum_{\tau} \vec{S}_{imp} \cdot \vec{S}_{0+\tau} + H_{so}
 \end{aligned} \tag{1}$$

where  $\tilde{c}_{i\sigma}$  is an electron operator within the Hilbert space excluding double occupancy, and  $\vec{S}_i$  and  $\mu$  are the spin-1/2 operator at a site  $i$  and the chemical potential, respectively. For the transfer integrals  $t_{ij}$  and the antiferromagnetic superexchange interaction  $J_{ij}$ , next-nearest-neighbor as well as nearest-neighbor terms are taken into account:  $t_{ij} = t \sum_{\tau} \delta_{i,j+\tau} + t' \sum_{\nu} \delta_{i,j+\nu}$ ,  $J_{ij} = J \sum_{\tau} \delta_{i,j+\tau} + J' \sum_{\nu} \delta_{i,j+\nu}$  with  $\tau = \pm\hat{x}, \pm\hat{y}$  and  $\nu = \pm\hat{x} \pm \hat{y}$ .

The impurity part consists of three terms: (i) potential scattering  $V_0$ , which is assumed to be in the unitary limit ( $V_0 \gg J, t$ ), (ii) exchange interaction  $J_0$  ( $\geq 0$ ) which acts between the impurity ( $\vec{S}_{imp}$ ;  $S_{imp} = 1$ ) and its nearest-neighbor sites, and (iii) spin-orbit interaction described by  $H_{so}$ . The model described by (i) and (ii) is essentially the same as the one studied by Poilblanc et al.<sup>12)</sup> We simplify the model by treating  $\vec{S}_{imp}$  as a classical spin,  $\langle \vec{S}_{imp}^z \rangle$ . The spin-orbit interaction  $H_{so}$  is given by

$$H_{so} = g \sum_{\sigma} \int d^2r \frac{1}{r^3} S_{imp}^z \tilde{c}_{\sigma}^\dagger(\vec{r}) [\vec{r} \times i\vec{\partial}]_z \tilde{c}_{\sigma}(\vec{r}). \tag{2}$$

in the continuum representation, and we transform this to that on a lattice by replacing the derivatives with discrete differences. In the actual calculations we take into account interactions only up to second-neighbor sites of the impurity for simplicity of numerical calculations.

We use the slave-boson method to enforce the condition of no double occupancy by introducing spinons ( $f_{i\sigma}$ ;

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fermion) and holons ( $b_i$ ; boson) ( $\tilde{c}_{i\sigma} = b_i^\dagger f_{i\sigma}$ ), and decouple this Hamiltonian by a mean-field approximation (MFA). In the following we consider only the case of zero temperature ( $T = 0$ ), so that holons are Bose condensed. Then the mean-field Hamiltonian is written in terms of spinons only,<sup>13)</sup>

$$\mathcal{H}_{MFA} = \sum_i \sum_j \Psi_i^\dagger \begin{bmatrix} W_{ij}^{(\uparrow)} & F_{ij} \\ F_{ji}^* & -W_{ji}^{(\downarrow)} \end{bmatrix} \Psi_j \quad (3)$$

with

$$\begin{aligned} W_{ij}^{(\sigma)} &= -(t_{ij}\delta + \frac{1}{2}J_{ij}\chi_{ji}^{(-\sigma)} + \frac{1}{4}J_{ij}\chi_{ji}^{(\sigma)}) \\ &+ \left[ \frac{\sigma}{2} \left( \sum_{\lambda} J_{i,i+\lambda} \langle S_{i+\lambda}^z \rangle + J_0 \langle S_{imp}^z \rangle \sum_{\tau} \delta_{i,0+\tau} \right) \right. \\ &\quad \left. - \mu + V_0 \delta_{i,0} \right] \delta_{i,j}, \\ F_{ij} &= -\frac{1}{2}J_{ij}\Delta_{ij} - \frac{1}{4}J_{ij}\Delta_{ji}, \\ \Psi_i^\dagger &= (f_{i\uparrow}^\dagger, f_{i\downarrow}^\dagger) \end{aligned} \quad (4)$$

where  $\delta$  is the doping rate, and the summations on  $i, j$  and  $\lambda$  are taken over all sites. Here the SC order parameter (OP),  $\Delta_{ij}$ , the hopping OP,  $\chi_{ij}$ , and the magnetization,  $\langle S_i^z \rangle$ , are defined as

$$\begin{aligned} \Delta_{ij} &= \langle f_{i\downarrow} f_{j\uparrow} \rangle, \quad \chi_{ij}^{(\sigma)} = \langle f_{i\sigma}^\dagger f_{j\sigma} \rangle, \\ \langle S_i^z \rangle &= \langle f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow} \rangle / 2. \end{aligned} \quad (5)$$

The SCOP with the definite symmetry can be constructed from  $\Delta_{ij}$ . For example  $d_{x^2-y^2}$ -wave OP ( $\Delta_d$ ) is defined as

$$\Delta_d(i) = (\tilde{\Delta}_{i,i+x} + \tilde{\Delta}_{i,i-x} - \tilde{\Delta}_{i,i+y} - \tilde{\Delta}_{i,i-y}) / 4 \quad (6)$$

with  $\tilde{\Delta}_{ij} = (\Delta_{ij} + \Delta_{ji}) / 2$  being the singlet-pairing OP. Here we do not exclude the spin-triplet pairing, and they actually can be finite as will be seen later.

In a uniform system without impurities only the  $d_{x^2-y^2}$ -wave OP is finite for the doping rate of our interest, i.e.,  $0.15 < \delta < 0.2$  (optimum and overdoped cases). In the presence of an impurity, however, OP with other symmetries can be mixed and we have to treat their spatial variations. In order to do this, we diagonalize the mean-field Hamiltonian by solving the following Bogoliubov de Gennes (BdG) equation<sup>14)</sup>

$$\sum_j \begin{bmatrix} W_{ij}^{(\uparrow)} & F_{ij} \\ F_{ji}^* & -W_{ji}^{(\downarrow)} \end{bmatrix} u_{jn} = E_n u_{in}, \quad (7)$$

where  $E_n$  and  $u_{in}$  are the energy eigenvalue and the corresponding eigenfunction, respectively. The unitary transformation  $\Psi_i = \sum_n u_{in} \Gamma_n$  diagonalizes the matrix  $\mathcal{H}_{MFA}$ , and conversely the OPs ( $\Delta_{ij}$ ,  $\chi_{ij}^{(\sigma)}$  and  $\langle S_i^z \rangle$ ) can be written in terms of  $E_n$  and  $u_{in}$ . These constitute the self-consistency equations which will be solved numerically in the following.<sup>15)</sup> We use  $J$  as a unit of energy (i.e.,  $J = 1$ ), and take  $t/J = 3$  throughout in this paper.

First we examine the effect of spin-exchange scattering. The potential scattering is also taken into account,

and the value  $V_0 = 100$  is used. For this value of  $V_0$  the scattering is in the unitary limit, since calculated hopping OPs ( $\chi$ ) connected to the impurity site vanish, indicating that electrons cannot hop to the impurity site. The spatial variations of the OPs for  $J_0 = 1$  are shown in Fig.1. It is seen that  $\Delta_d$  is suppressed near the impurity (Fig.1(a)), and the effect is strongest along the diagonals of the square lattice. This is due to the interference effects for momenta close to the gap nodes. In the region where  $\Delta_d$  is not uniform the extended  $s$ -wave OP ( $\Delta_s$ ; not shown) and the staggered magnetization (Fig.1(b)) are induced.<sup>16)</sup> The important point here is that the spin-triplet SCOPs,  $\Delta_{px}$  and  $\Delta_{py}$ , can also appear (Fig.1(c);  $\Delta_{py}$  has a similar behavior as  $\Delta_{px}$ ).  $\Delta_{px(y)}$  is defined as  $\Delta_{px(y)}(i) = (\Delta_{i,i+x(y)}^{(T)} - \Delta_{i,i-x(y)}^{(T)}) / 2$  where  $\Delta_{ij}^{(T)} = (\Delta_{ij} - \Delta_{ji}) / 2$  is the spin-triplet OP. In the presence of the magnetization there is the imbalance of the densities of spin-up and spin-down electrons. Then electron pairs cannot be formed in singlet channels only, and the spin-triplet components appear. We have also examined other values of  $J_0$ . The results are qualitatively the same, and the effect of spin-exchange scattering becomes larger (smaller) with increasing (decreasing)  $J_0$  as expected.

The above results can be understood more precisely using the Ginzburg-Landau (GL) theory. (The GL theory is not quantitatively valid except near  $T_c$ , but it can give qualitatively correct results.) The GL free energy in the continuum representation can be written as<sup>17)</sup>

$$\begin{aligned} \mathcal{F}_S &= \int d^2r \left( \sum_{j=d,s,px,py} [\alpha_j |\Delta_j|^2 + K_j |\vec{\partial} \Delta_j|^2 \right. \\ &+ g_j |\Delta_j|^2 \delta(r)] \\ &+ K_{ds} [(\partial_x \Delta_d)(\partial_x \Delta_s)^* - (\partial_y \Delta_d)(\partial_y \Delta_s)^* + c.c.] \\ &+ K_{dp} [\Delta_d \{ (\partial_x m) \Delta_{px}^* - (\partial_y m) \Delta_{py}^* \} m + c.c.] \\ &+ K_{sp} [\Delta_s \{ (\partial_x m) \Delta_{px}^* + (\partial_y m) \Delta_{py}^* \} m + c.c.] \end{aligned} \quad (8)$$

This  $\mathcal{F}_S$  is invariant under all symmetry operations for the square lattice and we have dropped higher order terms. Here we assume that all coefficients in  $\mathcal{F}_S$  are positive except  $\alpha_d$ . Due to the  $g_d$  term  $\Delta_d$  is suppressed and its gradient becomes finite over the range of the coherence length. Then  $\Delta_s$  is induced through the mixed gradient ( $K_{ds}$ ) term. The magnetization (denoted as  $m$ ) is assumed to be induced by the spin-exchange interaction and have staggered oscillations. When  $m$  and  $\Delta_d$  coexist and have spatial variations,  $p$ -wave OPs can occur due to  $K_{dp}$  term. In Fig.1  $\Delta_{px(y)}$  is finite where  $m$  is finite, and this result is consistent with the above argument. All induced OPs are real, since they are determined by bilinear coupling terms in  $\mathcal{F}_S$ . Note the proximity effect in a bilayer system composed of a  $d$ -wave superconductor and a (anti)ferromagnet can similarly induce  $p$ -wave OPs.<sup>18)</sup>

Next we consider the spin-orbit interaction. It was argued, based on a continuum model that the spin-

orbit impurity scattering in a  $d_{x^2-y^2}$ -wave superconductor can locally create a  $(d_{x^2-y^2} + id_{xy})$ -state which breaks time-reversal symmetry( $\mathcal{T}$ ).<sup>19,20,21</sup> This is because the  $(d_{x^2-y^2} + id_{xy})$ -state has an orbital moment and its coupling to the impurity spin can lower the energy of the system. We will show that in the  $t - J$  model a similar  $\mathcal{T}$ -breaking state can also appear. In order to see this we add small  $t'$  and  $J'$  terms, since the  $d_{xy}$ -component ( $\Delta'_d$ ) is the SCOP defined on the next-nearest-neighbor bonds. (Note  $J'$  of the order of  $J$  is necessary to have finite  $\Delta'_d$  in a system without impurities.) The spin-orbit coupling for Ni is estimated to be  $g/a \sim 30$  meV ( $a$  being the lattice constant).<sup>22,20</sup> Here we use a larger value  $g/a = 2.4J$  in order to compensate the fact that the long-range part of  $H_{so}$  is neglected in our calculation. ( $J$  is estimated to be  $J \sim 0.13$  eV, so our parameter is about 10 times larger than the realistic value.) We find that  $\Delta'_d$  (Fig2(a), (b)) as well as  $\Delta_s$  is actually induced, but not  $\langle S^z \rangle$  and  $\Delta_p$ . The induced OPs have nontrivial phase structure, namely the phases take values other than 0 or  $\pi$  (relative to  $\Delta_d$ ) and change as functions of the position. In particular  $\Delta'_d$  has a phase  $\pi/2$  along the diagonal direction where  $\Delta_d$  is strongly suppressed. This leads to a spontaneous current around the impurity (Fig.2(c)),<sup>23</sup> and the gap nodes in the  $d_{x^2-y^2}$ -wave SC state vanish due to the complex combination of SCOPs. These results are consistent with those in ref.19-21.<sup>24</sup> For the parameters used here the magnitude of the current is of the order of 10 nA near the impurity and is smaller in other regions, and the gap due to the induced OP is  $\sim 0.1$  meV. A rough estimate using Biot-Savart law gives a value of  $\sim 0.1$  G for a magnetic field produced by the current at the impurity site.

Now we examine the case where the spin-exchange and the spin-orbit interactions coexist. In this case we find a state which carries a spontaneous spin current (Fig.3) as well as usual charge current. The spin current is defined as the difference of the currents of spin-up and spin-down electrons. Its magnitude is typically  $10^{-2}$  of that of the charge current. The occurrence of the spin current is naturally understood as follows. Spontaneous currents can flow because the SCOPs have nontrivial phase structure due to the spin-orbit coupling  $g$ . In the presence of the spin-exchange interaction  $J_0$ , the magnetization  $m$  is finite, indicating that there is the imbalance of the densities of spin-up and spin-down electrons. Then the contributions to currents from electrons of opposite spins are not equal. Hence the spin current arises.

In summary we have studied the effect of a magnetic impurity in the superconducting state of the  $t - J$  model. The spin-exchange scattering induces spin-triplet SCOP near the impurity, while the spin-orbit interaction leads to a state with complex OPs and a spontaneous current. When both interactions coexist we find a spontaneous spin current as well as the usual charge current. In the present work the long-range part of the spin-orbit interaction and the vector potential are not included, the latter of which has a feedback effect of the spontaneous current on the electronic states.<sup>25</sup> Therefore the results presented here can be compared with experiments only

in a qualitative sense. If some element with a larger spin-orbit coupling can be doped in high- $T_c$  superconductors, there would be a larger (compared with Ni) possibility to realize a SC state with a spontaneous current and a full gap in the local density of states. The former (latter) could be detected by  $\mu$ SR (low-temperature STM) measurements.

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  - 14) See e.g., P.G. de Gennes: *Superconductivity of Metals and Alloys* (Addison-Wesley, 1989).
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  - 24) Since OPs other than  $\Delta_d$  and  $\Delta_s$  are also mixed, the symmetry of the state is not exactly  $(d_{x^2-y^2} + id_{xy})$ -wave in contrast to ref. 19-21.
  - 25) Besides the effects within the mean-field level, the magnetic field at the impurity site would weaken the Kondo effect, since the direction of  $\vec{S}_{imp}$  would be fixed to the  $z$ -axis.

**Fig. 1** Spatial variations of OPs for  $t = 3$ ,  $J = 1$ ,  $t' = J' = 0$ ,  $\mu = -0.339$  ( $\delta = 0.2$ ),  $V_0 = 100$ ,  $J_0 = 1$  and

$g = 0$ . The system size is  $25 \times 25$  sites, and an impurity is located at the center of the system. (a)  $\Delta_d$ , (b)  $\Delta_{px}$  and (c)  $\langle S_z \rangle$ . Note that all OPs are non-dimensional.

**Fig. 2** Spatial variations of (a)  $\text{Re}\Delta'_d$ , (b)  $\text{Im}\Delta'_d$ , and (c) the spontaneous current around the impurity. Parameters used are  $t = 3$ ,  $J = 1$ ,  $t' = -0.5$ ,  $J' = 0.2$ ,  $\mu = 0.4$  ( $\delta = 0.16$ ),  $V_0 = 100$ ,  $J_0 = 0$  and  $g = 2.4$ . The arrows in (c) indicate only the directions of the currents, but not the magnitudes.

**Fig. 3** Spin current around the impurity for  $t = 3$ ,  $J = 1$ ,  $t' = -0.5$ ,  $J' = 0.2$ ,  $\mu = -0.5$  ( $\delta = 0.189$ ),  $V_0 = 100$ ,  $J_0 = 0.6$  and  $g = 4.8$ . The arrows indicate only the directions of the currents, but not the magnitudes.

Fig1(a)

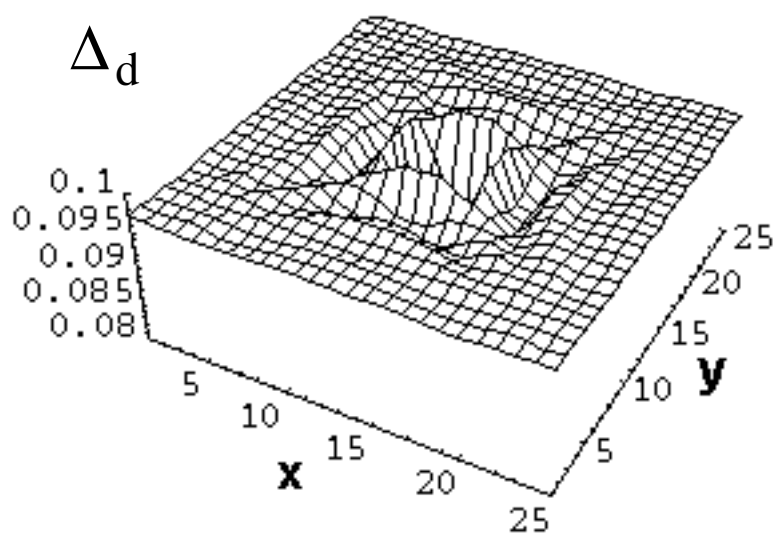


Fig1(b)

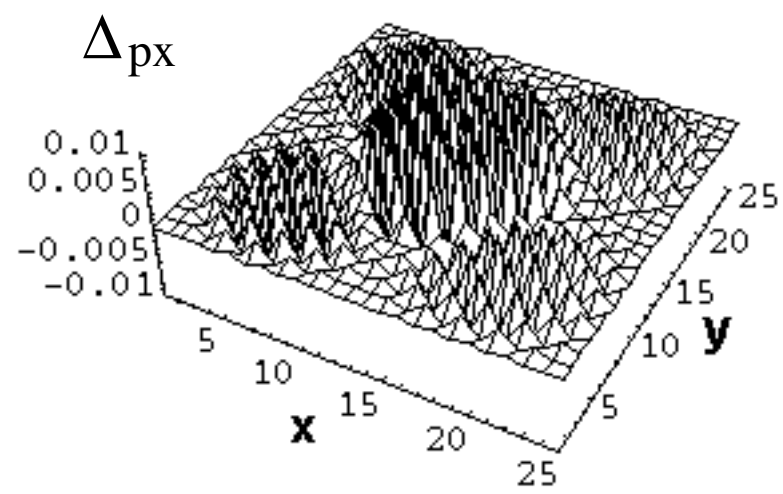
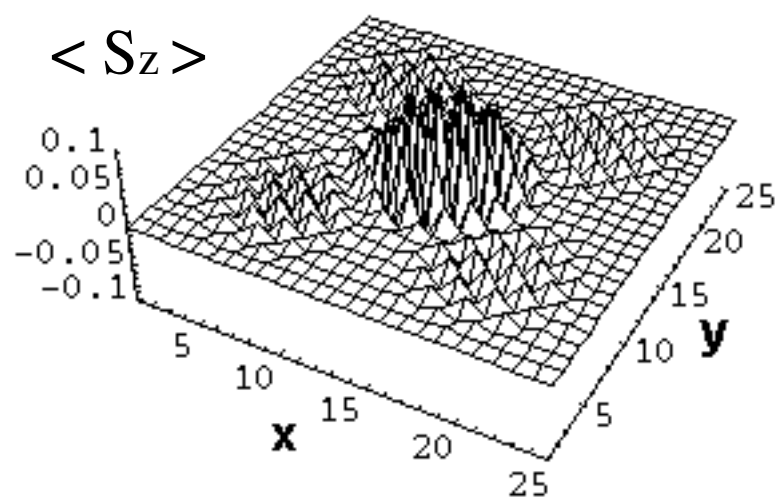


Fig1(c)



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Fig2(a)

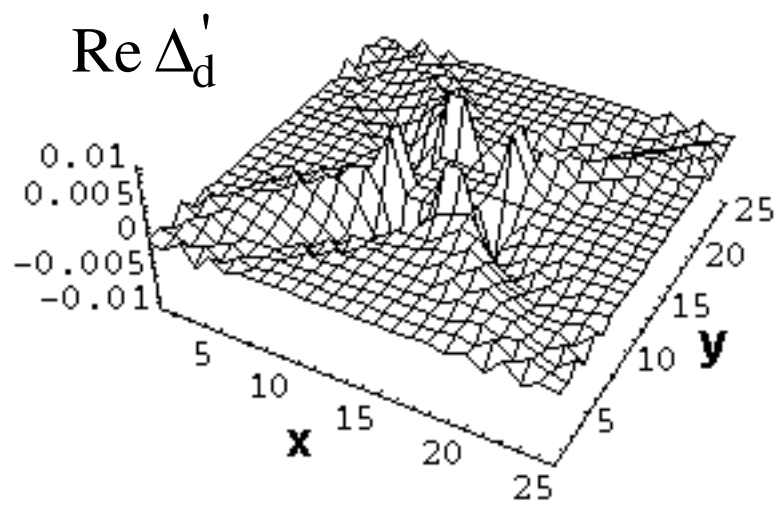
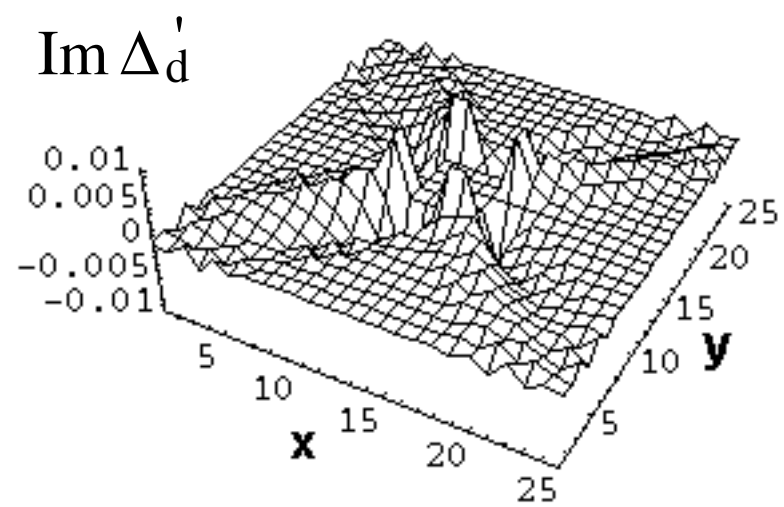


Fig2(b)



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